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# Accelerating Computation of the Nonlinear Mass by an Order of Magnitude

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## ABSTRACT

The nonlinear mass is a characteristic scale in halo formation that has wide-ranging applications across cosmology. Naively, computing it requires repeated numerical integration to calculate the variance of the power spectrum on different scales and determine which scales exceed the threshold for nonlinear collapse. We accelerate this calculation by working in configuration space and approximating the correlation function as a polynomial at  $r \leq 5 h^{-1}$  Mpc. This enables an analytic rather than numerical solution, accurate across a variety of cosmologies to 0.1–1% (depending on redshift) and 10–20× faster than the naive numerical method. We also present a further acceleration (40–80× faster than the naive method) in which we determine the polynomial coefficients using a Taylor expansion in the cosmological parameters rather than re-fitting a polynomial to the correlation function. Our acceleration greatly reduces the cost of repeated calculation of the nonlinear mass. This will be useful for MCMC analyses to constrain cosmological parameters from the highly nonlinear regime, e.g. with data from upcoming surveys. We make our `python` code publicly available at <https://github.com/akrolewski/NonlinearMassFaster>.

**Key words:** cosmology: theory—methods: numerical

## 1 INTRODUCTION

Computing the spatial scale on which the density fluctuations have variance of order unity is a common problem in cosmology. In bottom-up structure formation, fluctuations are small on large scales and become progressively larger on smaller scales. As the density fluctuations approach unity, Perturbation Theory (PT)-plus-biasing-based models of the clustering (Bernardeau et al. 2002) break down, and density fluctuations begin to collapse into dark matter halos.

The nonlinear scale  $R_{\text{NL}}$  is the characteristic scale at which these processes occur. Its technical definition is the scale at which the rms of the density field fluctuations,  $\sigma_R$ , reaches  $\delta_c = 1.686$  (Bryan & Norman 1998; Child et al. 2018), the linear-density threshold for spherical tophat collapse (Gunn & Gott 1972). The nonlinear scale  $R_{\text{NL}}$  can also be converted into a nonlinear mass  $M_{\text{NL}}$  by multiplying by the background density  $\rho_{\text{bgd}}$ .<sup>1</sup>

The nonlinear mass depends weakly on cosmology,

with the cosmology dependence arising from the small-scale power spectrum. Beyond the trivial dependence on the amplitude  $\sigma_8$  and the spectral slope  $n_s$ ,  $R_{\text{NL}}$  is most sensitive to  $\Omega_m$ . Increasing  $\Omega_m$  decreases the elapsed time in radiation domination. This leads to less suppression of small-scale modes entering the horizon during radiation domination, ultimately increasing small-scale power. The small-scale power spectrum is also sensitive to  $\Omega_b$ , both because baryons slow the growth of structure after matter-radiation equality but before decoupling (equation E-6 in Hu & Sugiyama 1996), and because the baryonic Jeans scale suppresses power at  $k \geq 300 h \text{ Mpc}^{-1}$ .

The nonlinear mass has broad applications across cosmology. Most importantly, it is the characteristic scale of halo formation in a scale-free power-law cosmology (Kravtsov & Borgani 2012) and is consequently the characteristic mass scale for self-similar scaling relations in galaxy clusters (Kaiser 1986; Bryan & Norman 1998; Norman 2010; Kravtsov & Borgani 2012). Although the nonlinear mass is

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<sup>1</sup> The background density may be either the matter density or the critical density, but does not contain a factor of  $\Delta_c \sim 200$ ,

the final-state overdensity of a virialized halo. This is because the nonlinear mass is defined with reference to the *linear* density threshold for the initial conditions of collapse.

not exactly the characteristic halo mass scale in a  $\Lambda$ CDM power spectrum, it is a good enough approximation that deviations from self-similar scalings are often parameterized in terms of it (Kravtsov & Borgani 2012). As an important determinant of halo formation, the nonlinear mass is the key scale in the halo growth rate (Wechsler et al. 2002), the concentration-mass relation (Child et al. 2018), assembly bias (Dalal et al. 2008), the mass-bias relation (Seljak & Warren 2004), and spin alignment between halos and filaments (Hahn et al. 2007a,b).

Due to these broad applications, the nonlinear mass plays a role in modeling nonlinear structure growth (Abazajian et al. 2005) and parameterizing the halo mass function to obtain  $\sigma_8$  (Seljak et al. 2005). Prompt calculation of the nonlinear mass will allow its inclusion in MCMC chains, enhancing cosmological constraints from the highly nonlinear regime, including weak lensing halo mass profiles (Umetsu et al. 2019) and cluster abundances (Bocquet et al. 2019). For instance, in the baryon-feedback model of Mead et al. (2015), which is included in the KiDS weak lensing analysis (Hilbrandt et al. 2018), the amplitude of feedback depends on the mass-concentration relation, which is in turn dependent on the nonlinear mass (Child et al. 2018).

We now outline how one might naively calculate the nonlinear mass, explain why this is inefficient, and sketch the approach of this work to accelerating the calculation. In the naive method, one computes a numerical integral for  $\sigma_R$  at each point in  $R$  traversed by a numerical root-finder solving the equation  $\sigma_R = \delta_c$ . The combination of the numerical integration and the root-finding makes  $R_{\text{NL}}$  slow to calculate.

In this work we present a scheme to greatly accelerate this calculation. Our method uses the algebraic solution of a cubic equation to determine  $R_{\text{NL}}$ , thereby bypassing both the numerical integration and the root-finding. In particular, we work in configuration space and fit a polynomial to the correlation function on small scales.  $\sigma_R$  is a compactly-supported integral over the correlation function, so these fitted coefficients immediately give us the integral's value as a cubic in  $R_{\text{NL}}$ . The equation  $\sigma_R = \delta_c$  can then be solved analytically. Our method is accurate to  $< 1\%$  for a variety of cosmologies, an order of magnitude faster than the standard method, and can be further accelerated by an additional  $4\times$  using a Taylor series to determine the polynomial coefficients of the correlation function.

All numerical work in this paper uses the best-fit cosmology from the *Planck* 2018 release (Planck Collaboration et al. 2018) with  $\Omega_m = 0.3096$ ,  $\Omega_b = 0.04897$ ,  $n_s = 0.9665$ ,  $\sigma_8 = 0.8102$ , and  $h = 0.6766$ .<sup>2</sup> Consistent with past work (e.g. Child et al. 2018), we use the linear power spectrum of cold dark matter plus baryons, since halos do not respond to neutrinos (Costanzi et al. 2013; Villaescusa-Navarro et al. 2014; Castorina et al. 2014, 2015).

<sup>2</sup> If one computes  $\sigma_8$  using our fiducial CDM-plus-baryons  $P(k)$ , one obtains 0.8138, in contrast to the *Planck* value of 0.8102, which is calculated for  $P(k)$  including CDM, baryons and neutrinos.

## 2 METHOD AND IMPLEMENTATION

In this section, we review the calculation of the variance of the density field in §2.1, present our algebraic method in §2.2, and show the solution to the cubic in §2.3.

### 2.1 Variance of the density field

The variance of the linear density field at a point  $\vec{x}$  and redshift  $z$  within a sphere of radius  $R$  is

$$\sigma_R^2(\vec{x}, z) = V_R^{-2} \int d^3\vec{r} d^3\vec{r}' \Theta(R - |\vec{r}|) \Theta(R - |\vec{r}'|) \delta_{\text{lin}}(\vec{x} + \vec{r}, z) \delta_{\text{lin}}(\vec{x} + \vec{r}', z). \quad (1)$$

$\Theta$  is a Heaviside function, unity where its argument is positive and zero otherwise. In 3-D, the Heaviside function of radius is simply a spherical tophat.  $V_R = 4\pi R^3/3$  is the volume of a sphere of radius  $R$ .

The statistical homogeneity of the density field implies translation invariance, and we may therefore write the average over  $\vec{x}$  as

$$\begin{aligned} \sigma_R^2(z) &\equiv \langle \sigma_R^2(\vec{x}, z) \rangle = \frac{1}{V} \int d^3\vec{x} \sigma_R^2(\vec{x}, z) \\ &= V_R^{-2} \int d^3\vec{r} d^3\vec{s} \Theta(R - |\vec{r}|) \Theta(R - |\vec{r} + \vec{s}|) \xi(s, z) \end{aligned} \quad (2)$$

where  $\vec{s} = \vec{r}' - \vec{r}$ , with  $\xi$  is the *linear* matter correlation function:

$$\xi(s, z) \equiv \int d^3\vec{x} \delta_{\text{lin}}(\vec{x} + \vec{r}, z) \delta_{\text{lin}}(\vec{x} + \vec{r} + \vec{s}, z) \quad (3)$$

and  $\delta_{\text{lin}}$  is the linear density field. To obtain the second equality in equation (2), we inserted equation (1) for  $\sigma_R(\vec{x}, z)$  and integrated over  $d^3\vec{x}$ , first using the definition of  $\xi$  in equation (3). By recasting equation (2) as a convolution we obtain

$$\sigma_R^2(z) = V_R^{-2} \int d^3\vec{s} \xi(s, z) [\Theta(R) \star \Theta(R)](\vec{s}) \quad (4)$$

where “star” denotes convolution.<sup>3</sup> The convolution inside the square brackets is evaluated at an offset  $\vec{s}$  and is itself an integral over the dummy variable  $\vec{r}$ ; for clarity we have suppressed this latter argument. Equation (4) shows that the variance is thus just the integral of the correlation function against a kernel given by the convolution of two spherical tophats at an offset  $\vec{s}$ .

The overlap of the two spheres forms a lens. Consequently we can evaluate the convolution using the formula for the volume of a lens produced by overlapping two spheres of radius  $R$ , offset from each other by  $s$  (Weisstein 2017a):

$$[\Theta(R) \star \Theta(R)](\vec{s}) = V_{\text{lens}}(s; R) = \frac{\pi}{12} (4R + s)(2R - s)^2. \quad (5)$$

In the limit  $s \rightarrow 0$ , i.e. when the two spheres share a common center, this expression recovers the volume of a sphere.

<sup>3</sup> This formula offers a geometric way to show that the overlap integral of two spherical Bessel functions  $j_1(kR)j_1(ks)$  scales as the volume of the lens formed by the overlap of two spheres.

Inserting equation (5) in equation (4) yields

$$\begin{aligned}\sigma_R^2(z) &= 4\pi V_R^{-2} \int_0^{2R} s^2 ds \xi(s, z) V_{\text{Lens}}(s; R) \\ &= 4\pi V_R^{-2} \int_0^{2R} s^2 ds \xi(s, z) (4R + s)(2R - s)^2 \\ &= \frac{\pi^2 R^3}{3V_R^2} \int_0^2 y^2 dy \xi(yR, z) (4R + yR)(2R - yR)^2.\end{aligned}\quad (6)$$

To obtain the third equality we changed variables to  $s = yR$ ,  $s^2 ds = R^3 y^2 dy$ . Simplifying the last line we obtain the formula of Zehavi et al. (2005), quoted there without proof but obtained by direct integration.<sup>4</sup>

$$\sigma_R^2(z) = \int_0^2 dy y^2 \xi(yR, z) K(y), \quad (7)$$

with

$$K(y) = \left(3 - \frac{9y}{4} + \frac{3y^3}{16}\right). \quad (8)$$

We will refer to  $K(y)$  as defined in equation (8) as the “kernel” for the remainder of this work. We plot the components of equation (7) in Figure 1, including the kernel and  $y^2 \xi(yR, z = 0)$  for different values of  $R$ . Since  $K(y)$  is nearly zero at  $y > 1.5$  and  $y^2 \xi(yR)$  is nearly zero at  $y < 0.5$ , much of the integral comes from intermediate values of  $y$ .

## 2.2 Solving for the nonlinear scale

The standard approach to computing  $R_{\text{NL}}$  is to use the Convolution Theorem to perform the convolution (equation 4) as a product in Fourier space, i.e.

$$\sigma_R^2(z) = \int \frac{k^2 dk}{2\pi^2} \left[ \frac{3j_1(kR)}{kR} \right]^2 P(k, z), \quad (9)$$

where the quantity in square brackets is the square of the Fourier Transform of a spherical tophat. One would then use numerical root-finding to solve the equation  $\sigma_{R_{\text{NL}}}(z) = \delta_c = 1.686$ .

Our method evaluates  $\sigma_R^2$  from equation (7) in configuration space and fits a low-order polynomial to the small-scale correlation function, leading to an analytic integral that enables algebraic calculation of  $R_{\text{NL}}$ . This is an order of magnitude faster than the standard method to compute  $R_{\text{NL}}$  from numerical integrals of the power spectrum.

Our method offers two advantages that substantially accelerate the calculation of the nonlinear scale. First, the configuration space integral is easier to handle than the Fourier space integral, which has an infinite upper bound and BAO wiggles which require a larger number of  $k$  steps for accurate sampling. Second, the correlation function on small scales is smooth and can be approximated by a low-order polynomial (Figure 2). This allows the  $\sigma_R^2$  integral to be evaluated analytically and  $R_{\text{NL}}$  then computed algebraically.

To obtain an analytic expression for  $\sigma_R^2$  for a polynomial correlation function, we start with the center line in

equation (6); separating the integrals term by term we find

$$\begin{aligned}\sigma_R^2(z) &= D^2(z) R^{-3} \left\{ 3 \int_0^{2R} ds s^2 \xi(s) - \frac{9}{4R} \int_0^{2R} ds s^3 \xi(s) \right. \\ &\quad \left. + \frac{3}{16R^3} \int_0^{2R} ds s^5 \xi(s) \right\},\end{aligned}\quad (10)$$

where we explicitly separate the redshift-dependent piece of the linear correlation function, the square of the linear growth factor  $D^2(z)$ , and hereafter use  $\xi(s)$  to mean  $\xi(s, z = 0)$ .

We perform the integral in equation (10) analytically by expanding  $s^2 \xi(s)$  as a polynomial:

$$s^2 \xi(s) = \sum_{n=0}^{n_{\text{max}}} c_n s^n. \quad (11)$$

We chose a polynomial because it allows the integral in equation (7) to be done analytically and provides a good fit to the correlation function over the restricted range required ( $s \leq 5 h^{-1}$  Mpc).

Inserting the expansion (11) into equation (10) and performing the integrals, we obtain the following expression for  $\sigma_R^2$ , which we set equal to  $\delta_c^2$ :

$$\begin{aligned}\sigma_{R_{\text{NL}}}^2(z) &= D^2(z) \sum_{n=0}^{n_{\text{max}}} c_n R_{\text{NL}}^{-3} \left\{ 3 \frac{2^{n+1}}{n+1} R_{\text{NL}}^{n+1} - \frac{9}{4R_{\text{NL}}} \frac{2^{n+2}}{n+2} R_{\text{NL}}^{n+2} \right. \\ &\quad \left. + \frac{3}{16R_{\text{NL}}^3} \frac{2^{n+4}}{n+4} R_{\text{NL}}^{n+4} \right\} \\ &= D^2(z) \sum_{n=0}^{n_{\text{max}}} 2^{n+1} c_n R_{\text{NL}}^{n-2} \left\{ \frac{9}{n^3 + 7n^2 + 14n + 8} \right\} = \delta_c^2.\end{aligned}\quad (12)$$

We transform equation (12) from a sum of inverse powers to a polynomial by multiplying through by  $R_{\text{NL}}^2$ :

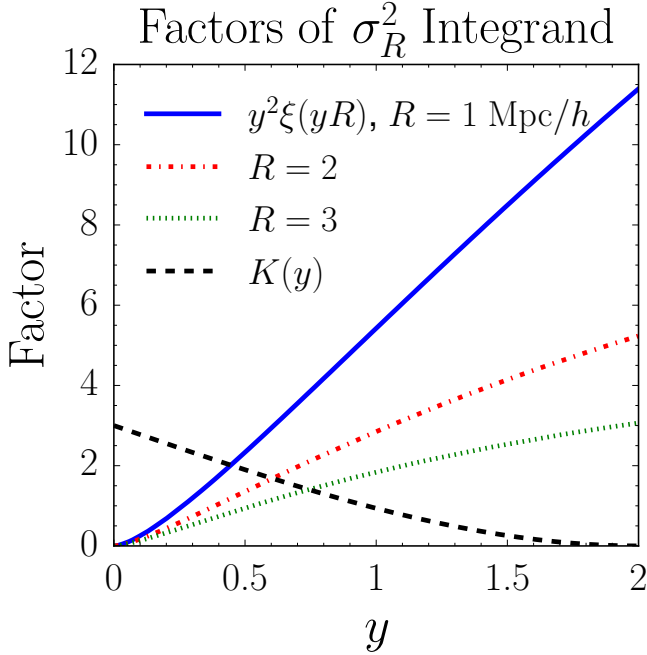
$$\frac{R_{\text{NL}}^2 \delta_c^2}{D^2(z)} = \sum_{n=0}^{n_{\text{max}}} 2^{n+1} c_n R_{\text{NL}}^n \left\{ \frac{9}{n^3 + 7n^2 + 14n + 8} \right\} \quad (13)$$

Quartics and lower-order polynomials have a closed form solution, but quintics and higher-order polynomials do not (this is known as the Abel-Ruffini theorem). Therefore, if  $n_{\text{max}} \leq 4$ , we can solve in closed form for  $R_{\text{NL}}$ .

We find that  $n_{\text{max}} = 3$  is sufficient to reproduce  $s^2 \xi(s)$  to percent-level accuracy (Figure 2), implying that an algebraic solution for  $R_{\text{NL}}$  exists. While Figure 2 only shows the fit to the correlation function in the *Planck* 2018 cosmology,  $s^2 \xi(s)$  can be approximated equally well by a cubic across a wide range of cosmologies. Because the cubic provides a good fit across a wide range in  $s$ , the analytic approximation of  $\sigma_R$  from integrating equation (10) provides a very good match to the numerical solution from the Fourier-space integral at  $R > 0.5 h^{-1}$  Mpc at  $z = 0$  (Figure 3).

We found that the cubic provides the best balance between simplicity and accuracy: a quadratic approximation is considerably less accurate, whereas a quartic offers only minimal improvement. Other possibilities, such as omitting the constant and linear terms or requiring the constant term to be positive, degrade the accuracy of the fit. While a piecewise function (e.g. a smoothing spline) can reproduce  $s^2 \xi(s)$  to arbitrary accuracy, the upper bounds in the integrals in equation (10) are no longer linear multiples of  $R$ , and thus

<sup>4</sup> D. Eisenstein, personal communication.

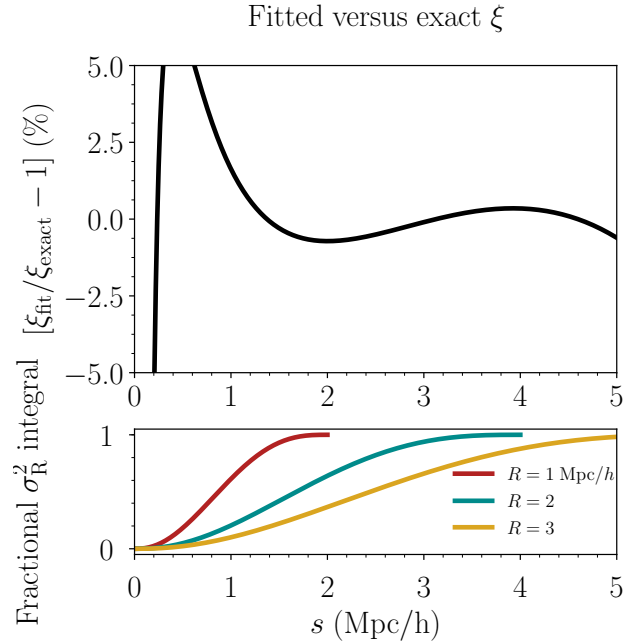


**Figure 1.** Different pieces of the integral (7). The dashed black line is the kernel  $K(y)$  defined in equation (8); and the short-dashed, dot-dashed and solid lines (various colors) are  $y^2\xi(yR)$  at  $R = 1, 2$ , and  $3$  Mpc/h. The dominant contribution to  $\sigma_R^2$  comes from intermediate  $y$ , where both  $K(y)$  and  $y^2\xi(yR)$  are nonzero.

contribute an  $R^{-6}$  term in equation (12). If  $n_{\max} \geq 1$ , this yields a 5th-order polynomial with no analytic solution in equation (14).

Equation (11) must approximate  $s^2\xi(s)$  well at  $s < 2R_{\text{NL}}(z)$ , since this is the upper bound of the integral in equation (10). To avoid the circularity of requiring  $R_{\text{NL}}$  to fit the  $c_n$ , we fit the  $c_n$  to  $s < 1.9R_{\text{NL, fid}}(z)$ , where  $R_{\text{NL, fid}}$  is  $R_{\text{NL}}$  in the fiducial *Planck* 2018 cosmology. We empirically find that using an upper cutoff of  $1.9R_{\text{NL, fid}}(z)$  leads to 20% better accuracy than using  $2R_{\text{NL, fid}}(z)$ . This slightly up-weights smaller and intermediate scales which contribute more to the  $\sigma_R^2$  integral (bottom panel of Figure 2).

Allowing the fitting range (and thus the  $c_n$ ) to vary in redshift is critical, because the error on the cubic increases greatly at small  $s$ : this is the sharp drop in the signed deviation between the correlation function and the cubic fit at  $s \leq 0.5 h^{-1}$  Mpc in Figure 2 (or equivalently, the downturn in  $\sigma_R^2$  at  $R > 1 h^{-1}$  Mpc in Figure 3). If we calculated  $R_{\text{NL}}(z=6)$  using  $c_n(z=0)$ , we would be primarily using scales where the cubic provides an extremely poor fit to  $s^2\xi(s)$ , leading to a severe loss of accuracy. Instead, we fit over a very restricted  $s$  range at  $z=6$ , ensuring an accurate fit over the vast majority of the relevant range in  $s$ . Because of this rescaling in  $R_{\text{NL, fid}}(z)$ , Figures 2 and 3 at  $z=0$  are very similar to the equivalent figures at high redshift, except that the  $s$  ( $R$ ) axis will be rescaled by  $R_{\text{NL, fid}}(z)/R_{\text{NL, fid}}(z=0)$ .



**Figure 2.** *Top*— Difference between  $s^2\xi_{\text{lin}}(z=0)$  and the third-order polynomial fit to it. The differences in fitting quality are negligible among different cosmologies. We recover the exact correlation function to rather high accuracy, generally sub-percent over most of its domain; larger errors occur at small scales which contribute little to the fractional  $\sigma_R^2$  integral, as shown in the bottom panel. *Bottom*— Fractional buildup of  $\sigma_R^2$  (equation 7) as a function of  $s \equiv yR$ . Since the integral extends to  $y=2$ , the curves cut off at respectively  $yR=2, 4$  and  $6$  for  $R=1, 2$ , and  $3$  Mpc/h. For a wide range in  $R$ , the integral turns out to be most sensitive to exactly the region in which our fit performs best,  $1 < s < 5 h^{-1}$  Mpc.

### 2.3 Detailed solution of the cubic

In this section we explicitly show how one obtains  $R_{\text{NL}}$  algebraically. Evaluating equation (13) with  $n_{\max} = 3$  yields

$$\frac{9}{4}R^{-2}c_0 + \frac{6}{5}R^{-1}c_1 + c_2 + \frac{36}{35}Rc_3 = \frac{\delta_c^2}{D^2(z)}. \quad (14)$$

To simplify what follows, we define coefficients  $a_i$  that incorporate both the  $c_n$  and their numerical pre-factors in equation (14), as

$$a_0 = \frac{9c_0}{4}, \quad a_1 = \frac{6c_1}{5}, \quad a_2 = c_2, \quad a_3 = \frac{36c_3}{35}. \quad (15)$$

We now rewrite equation (14) in standard cubic form

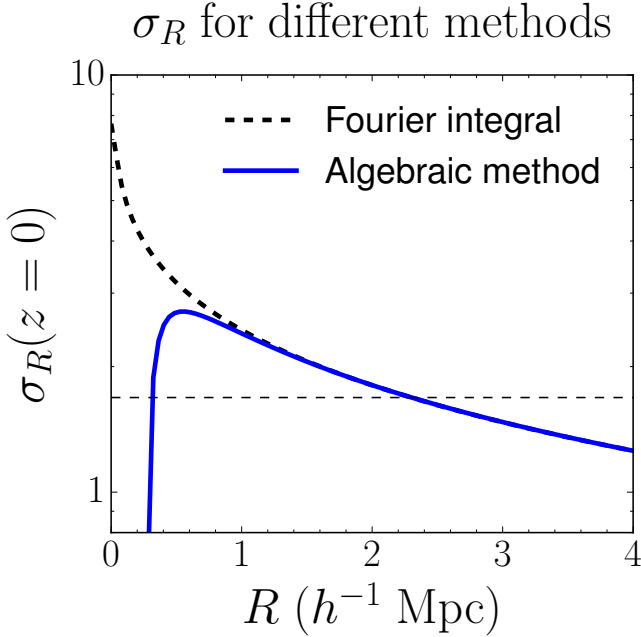
$$R^3 + a_2R^2 + a_1R + a_0 = 0 \quad (16)$$

with the  $a_i$  given as

$$a_0 = \frac{a_0}{a_3}, \quad a_1 = \frac{a_1}{a_3}, \quad a_2 = \frac{a_2 - 1/D(z)^2}{a_3}. \quad (17)$$

We can obtain the solution using Cardano's formula for the cubic (Weisstein 2017b). We find the roots  $R_i$  as:

$$R_1 = -\frac{1}{3}a_2 + (S + T),$$



**Figure 3.** Comparison between exact  $\sigma_R$  from the Fourier integral (blue; equation 9) and our algebraic method (black; equation 14). Both calculations are done at  $z = 0$ ; results for  $\sigma_R(z)$  will be very similar except that the horizontal axis will be scaled by  $R_{\text{NL, fid}}(z)/R_{\text{NL, fid}}(z = 0)$ . The thin black dashed line gives  $\sigma_R = \delta_c = 1.686$ ; thus  $R_{\text{NL}}$  is where the thicker curves cross the dashed line. While the solid and dashed curves disagree at small scales, the agreement is almost perfect near where  $\sigma_R = 1.686$ .

$$R_2 = -\frac{1}{3}\alpha_2 - \frac{1}{2}(S + T) + \frac{1}{2}i\sqrt{3}(S - T),$$

$$R_3 = -\frac{1}{3}\alpha_2 - \frac{1}{2}(S + T) - \frac{1}{2}i\sqrt{3}(S - T). \quad (18)$$

We define the auxiliary variables  $Q$ ,  $R$ ,  $D$ ,  $S$ , and  $T$  as

$$Q \equiv \frac{3\alpha_1 - \alpha_2^2}{9}, \quad R \equiv \frac{9\alpha_2\alpha_1 - 27\alpha_0 - 2\alpha_2^3}{54},$$

$$D \equiv Q^3 + R^2, \quad S \equiv \sqrt[3]{R + \sqrt{D}}, \quad T \equiv \sqrt[3]{R - \sqrt{D}}. \quad (19)$$

We choose the real and positive root. Note that despite the presence of  $i$  in  $R_2$  and  $R_3$ , they need not be complex because  $S$  and  $T$  are also complex and can render the factor involving  $i$  real overall.

### 3 NUMERICAL IMPLEMENTATION

To obtain the nonlinear scale using the method outlined in §2.2 and §2.3, we first need the linear correlation function. We obtain the correlation function by transforming the linear power spectrum from CAMB (Lewis et al. 2000; Howlett et al. 2012).<sup>5</sup> We use 800 logarithmically-spaced sample points per decade over the range  $k = 10^{-3}$  to  $10^4$

$h \text{ Mpc}^{-1}$ . To transform from  $P(k)$  to  $\xi(s)$  we use  $2 \times 10^4$   $s$ -points evenly spaced between  $s = 0$  and  $5 h^{-1} \text{ Mpc}$ . For consistency with past work (Child et al. 2018), we use the power spectrum of baryons plus CDM in our numerical implementation, but the method is general and can accept an arbitrary linear power spectrum as input.

For the timing tests in §4, we find  $R_{\text{NL}}$  using optimized implementations of both the algebraic method and the numerical integral methods in Fourier and configuration space. We aim to achieve 0.01% accuracy on  $R_{\text{NL}}$  for the numerical integral methods in both Fourier and configuration space.

The most time-consuming part of our implementation of the polynomial method is solving for the polynomial coefficients  $c_n$ . We use 1000 sampling points for the correlation function and determine  $c_n$  via linear least-squares. The relevant operations are vectorized so the performance is not highly sensitive to the number of sampling points. Consequently we can choose 1000 points to preserve accuracy yet not pay much price in speed. The rate-limiting step is matrix inversion in the linear least squares fitting; to speed this up, we take advantage of the fact that the relevant matrix is symmetric, as it is the product of the Vandermonde matrix and its transpose. We solve the least squares equation using the `lapack` linear algebra package routine `dpotrs` (double-precision positive triangular matrix solve), which uses Cholesky decomposition to efficiently invert a symmetric matrix (Press et al. 2002).<sup>6</sup> This approach is considerably faster than the `numpy` least-squares package, both by eliminating `numpy` overheads and by using a faster method specifically appropriate for symmetric matrices.

As an alternative to the time-consuming determination of the polynomial coefficients, we determine  $c_n$  using a Taylor expansion in the cosmological parameters ( $\Omega_m$ ,  $\Omega_b$ ,  $n_s$ ) centered on the fiducial cosmology. The dependence on  $\sigma_8$  is trivial, as it just rescales the polynomial coefficients by a multiplicative factor. This expansion assumes the mapping of parameters to power spectra appropriate for a CDM cosmology; modifications to the transfer function, e.g. by warm dark matter or oscillations in the inflationary potential, will change this mapping and require fitting the polynomial coefficients rather than using the Taylor series.

To compute the Taylor expansion for each  $c_n$ , we first compute correlation functions and  $c_n$  for four cosmologies per parameter varied ( $\Omega_m$ ,  $\Omega_b$  and  $n_s$ ): two with the parameter varied by  $\pm 1\sigma$  from the *Planck* 2018 best-fit value (with  $\sigma = 0.0056$ , 0.001 and 0.0038, respectively) and two with the parameter varied by  $\pm 5\sigma$ . Then for each  $c_n$  and parameter  $p$ , we fit a line  $c_n(p)$  with the intercept fixed to reproduce  $c_n$  in the fiducial cosmology. This allows us to achieve a good fit for a broad range of cosmologies away from the *Planck* best-fit cosmology.

We must re-fit  $c_n$  at each  $z$  to ensure an accurate fit over most of the relevant range in scale (§2.2). Therefore, we must also determine the Taylor coefficients as a function of redshift. We measure the first-order Taylor coefficients for the three parameters for 60 sampling redshifts spaced at  $\Delta z = 0.1$  between  $z = 0$  and 6. We determine the Taylor coefficients at arbitrary  $z$  using a step function taking each  $z$  to the nearest  $\Delta z = 0.1$  grid point less than  $z$ .

<sup>5</sup> <http://camb.info>

<sup>6</sup> <http://www.netlib.org/lapack/>



Once the polynomial coefficients are fit, finding the non-linear scale is straightforward, requiring only algebraic operations. Nevertheless, we make a number of optimizations to the code implementing this. We store intermediate calculations to reduce computational expense, use only built-in `python` functions or functions from the `math` library, and use decimals rather than fractions wherever possible to avoid an additional division. We also optimize the performance of the naive method, with numerical integration and root-finding (in either Fourier or configuration space), in order to provide a fair comparison.

For the configuration space integral (equation 7), we use 50 sampling points in  $y$  and pre-compute the kernel since it does not change from iteration to iteration of the root-finding. We evaluate the integral using direct summation over the 50 points in  $y$ . We find that this gives sufficient accuracy (better than  $10^{-4}$ ) and is considerably faster than second-order methods such as Romberg integration. As with fitting the polynomial coefficients, the scaling of the integral is relatively insensitive to the number of sampling points due to the vectorization of most operations. Therefore, our results will not change much if the number of sampling points changes.

We use the `scipy` implementation of Brent’s method (`brentq`) (Brent 1973) to perform the root-finding, with the initial range between 0 and  $5 h^{-1}$  Mpc, comfortably bracketing  $R_{\text{NL}}$  in all plausible cosmologies. We use this method because we find it to be the most robust for root-finding.<sup>7</sup>

We follow largely the same procedure to evaluate the integral in Fourier space (equation 9), except that here, we find that first-order summation is inaccurate and instead use the second-order trapezoid rule. We also downsample the original  $k$ -space grid to achieve better performance, finding that 180 logarithmically-spaced points between  $k_{\text{min}} = 10^{-3} h \text{ Mpc}^{-1}$  and  $k_{\text{max}} = 10^4 h \text{ Mpc}^{-1}$  are adequate. Again, the scaling with number of points is weak, so our timings do not depend strongly on the number of sampling points chosen.

Finally, we make our `python` code publicly available at <https://github.com/akrolewski/NonlinearMassFaster>.

## 4 RESULTS AND DISCUSSION

We measure the accuracy of our algorithm for finding  $R_{\text{NL}}$  compared to numerical integration of equation (9) using a large number of sampling points in  $k$ . We also measure the speed of our algorithm, both when we fit the coefficients  $c_n$  for every cosmology, and when we use a Taylor expansion to calculate  $c_n$  for cosmologies sufficiently close to *Planck* 2018. We compare the timing of our algorithm to optimized versions of the numerical integration and root-finding method in both configuration and Fourier space. We find the algebraic method is accurate to 0.1–1% in mass and offers a factor of 10–20 speedup over the naive method, while the Taylor series method is accurate to 1–10% in mass and 40–80× faster than the naive method.

<sup>7</sup> Newton-Raphson root-finding is 30–50% faster than Brent’s method, but less robust as the root-finding has no bounds. Therefore, for higher  $z$  where  $R_{\text{NL}}$  becomes small, the root finder may attempt to evaluate  $\sigma_R$  at negative  $R$ , which is of course unphysical.

Name	$\sigma_8$	$\Omega_m$	$\Omega_b$	$n_s$
$\sigma_8 + 0.06$	0.8702	0.3096	0.04897	0.9665
$\sigma_8 - 0.06$	0.7502	—	—	—
<i>Planck</i> 2018	0.8102	—	—	—
C1	—	0.3129	0.0490	0.9669
C2	—	0.3185	0.0498	0.9676
C3	—	0.3145	0.0479	0.9616
C4	—	0.3086	0.0507	0.9591
C5	—	0.3004	0.0504	0.9663

**Table 1.** Cosmologies used to test our method. The default cosmology is *Planck* 2018, and the cosmologies C1–C5 are chosen by randomly drawing  $\Omega_m$ ,  $\sigma_8$  and  $n_s$  from a uniform distribution of width  $\pm 2\sigma$  centered on the *Planck* 2018 values. Dashes indicate that a given parameter is unchanged from the row above. Accuracy and timing results for these cosmologies are given in Figures 4 and 5.

We use `python` 3.5.2, with `numpy` 1.17.1 and `scipy` 1.3.1. Timing tests are performed on a dual core 1.7 GHz Intel Core i5 processor.<sup>8</sup> We use seven cosmologies to test our method. We start with two where  $\sigma_8$  is varied by  $\pm 0.06$  from its best-fit *Planck* 2018 value, matching the tension between *Planck* and the low-redshift measurement from KiDS (Hilbrandt et al. 2018).<sup>9</sup> We also use five test cosmologies with  $\Omega_m$ ,  $\Omega_b$  and  $n_s$  drawn from a random uniform distribution between  $2\sigma$  less than and  $2\sigma$  greater than the *Planck* 2018 best-fit value for each parameter. These explore a range in which many recent simulations lie (Klypin et al. 2016; Klypin & Prada 2018; Villaescusa-Navarro et al. 2019). The parameters for these test cosmologies are given in Table 1.

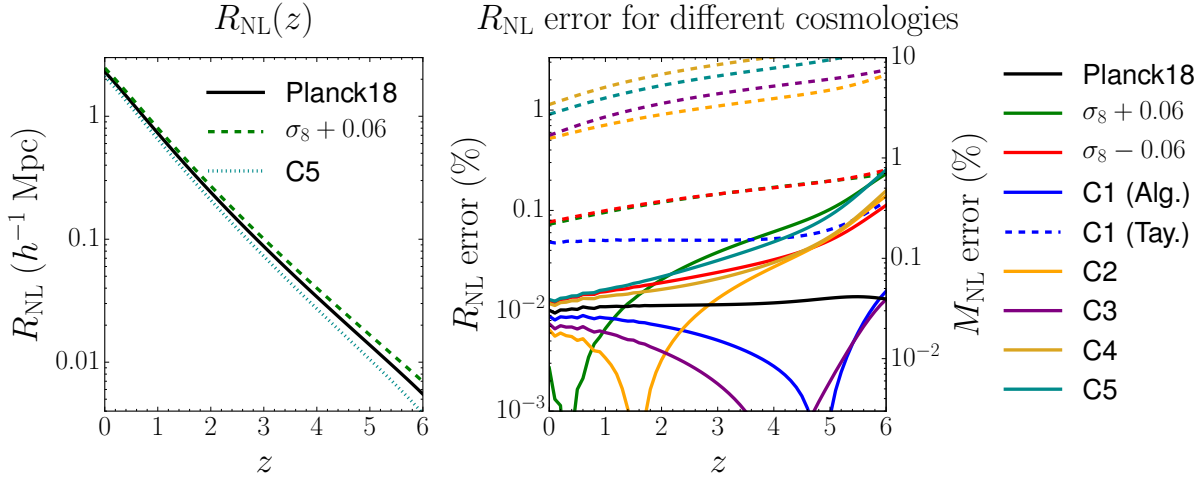
Our fiducial method, in which we re-fit the coefficients for each input power spectrum, is accurate to better than 0.3% in  $R_{\text{NL}}$  (1% in  $M_{\text{NL}}$ ) at  $0 < z < 6$  for all seven of these test cosmologies (Figure 4). If we instead use a Taylor expansion about the *Planck* 2018 cosmology to generate the coefficients, the accuracy is somewhat worse, between 1% and 10% in mass. Therefore, the Taylor series method may be adequate at  $z \sim 0$ , where it offers 1% accuracy in  $R_{\text{NL}}$  and 3% accuracy in mass, but at higher redshifts it is likely best to explicitly re-fit the polynomial coefficients, depending on the accuracy demands of one’s application.

We plot  $R_{\text{NL}}(z)$  in the left panel of Figure 4 for the *Planck* 2018 cosmology ( $R_{\text{NL},\text{fid}}$ ) and for the two cosmologies with the largest deviation in  $R_{\text{NL}}(z)$ , C5 and  $\sigma_8 + 0.06$ . At  $z = 0$ ,  $R_{\text{NL}}$  in  $\sigma_8 + 0.06$  (C5) is 7% higher (8% lower) than  $R_{\text{NL},\text{fid}}$ , increasing to 25% higher (30% lower) at  $z = 6$ .  $R_{\text{NL}}$  is very small at high redshift, with  $R_{\text{NL}}(z = 6) \approx 0.005 h^{-1} \text{ Mpc}$ . This does not imply that the  $z = 6$  linear power spectrum is valid out to  $k_{\text{NL}} = 2\pi/0.005 \approx 1000 h \text{ Mpc}^{-1}$ . Rather, the  $k$  at which the linear and nonlinear power spectra deviate is smaller than  $k_{\text{NL}}$  by a factor of a few.

Because we use  $R_{\text{NL}}$  in the *Planck* 2018 cosmology to set

<sup>8</sup> This is a similar architecture to the Cori Haswell nodes at the National Energy Research Supercomputing Center (NERSC) (see <https://docs.nersc.gov/systems/cori/>), hence the performance numbers outlined here can plausibly be scaled to get a rough estimate for the performance on a typical recent HPC system.

<sup>9</sup> Weak lensing measurements are sensitive to the parameter combination  $S_8 = \sigma_8 \sqrt{\Omega_m}/0.3$ . KiDS measures  $S_8 = 0.737^{+0.040}_{-0.036}$  (Hilbrandt et al. 2018); if  $\Omega_m$  is fixed to 0.3, this implies  $\sigma_8 \sim 0.75$ .



**Figure 4.** Left:  $R_{\text{NL}}(z)$  for the *Planck* 2018 cosmology (black), and the C5 and  $\sigma_8 + 0.06$  cosmologies (dark cyan, dotted; green, dashed), which have the largest discrepancy with the *Planck* 2018  $R_{\text{NL}}$ . Right: Absolute value of the error on  $R_{\text{NL}}$  (left-hand vertical axis) and the nonlinear mass (right-hand vertical axis;  $3\times$  the  $R_{\text{NL}}$  error) as a function of redshift. We compare the accuracy for our 7 test cosmologies using the fiducial method, where we re-fit the coefficients to each cosmology (solid, colored curves). We also show the Taylor series method, where we use a Taylor expansion about the *Planck* 2018 cosmology to generate the coefficients (dashed curves). Each color stands for one of the 7 test cosmologies, and the line style indicates whether we re-fit the coefficients or determine them from the Taylor series. Cosmological parameters are given in Table 1. At  $z \sim 1.5$ , the error on  $R_{\text{NL}}$  for C2 changes sign from positive to negative, leading to the zero-crossing feature in the golden curve (and likewise for the green, purple and blue curves at various redshifts).

the fitting range, the accuracy of our method should degrade as the cosmology varies. However, for certain cosmologies and redshift ranges ( $\sigma_8 - 0.06$  at  $z < 1$ , C2 at  $z < 3$ , and C1 and C3 at  $z < 6$ ), the accuracy is *better* than the accuracy for *Planck* 2018. This is because the mismatch between  $R_{\text{NL}}$  in these cosmologies and  $R_{\text{NL, fid}}$  is actually beneficial, since the (cosmology-dependent) optimal upper bound is not exactly  $1.9R_{\text{NL}}$ . For these cosmologies and redshifts,  $1.9R_{\text{NL, fid}}$  approaches the optimal upper bound at the points where the error approaches zero (e.g.  $z \approx 1.5$  for C2).

The  $R_{\text{NL}}$  error for many of the test cosmologies increases at higher redshift. This is because  $R_{\text{NL}}$  is smaller at high redshift, and thus sensitive to the linear power spectrum at higher  $k$  where the power spectrum is more cosmology dependent.<sup>10</sup> This means that the disagreement between  $R_{\text{NL}}$  and  $R_{\text{NL, fid}}$  is larger, leading to a suboptimal fitting range and inaccurate polynomial coefficients. As a consequence, if we instead solve for the scale where  $\sigma_R = 1$  (e.g. Norman 2010), our method will be more accurate because this scale is larger and less dependent on high  $k$ , yielding a better fitting range and more accurate polynomial coefficients.

We compare the timing for the algebraic method and the numerical integral plus root-finding method in both configuration and Fourier space (Figure 5). If we fit the polynomial coefficients to the correlation function, our method is faster than the naive Fourier space method by a 10–20 $\times$ ; if we generate the polynomial coefficients from a Taylor expansion about the *Planck* 2018 cosmology, our method is 40–80 $\times$  faster than the Fourier space method. Some of these gains are from working in configuration space rather than in

Fourier space, where the integral is easier to evaluate. However, our algebraic method is still a factor of 2–4 $\times$  faster than the naive method in configuration space.

The timing of the naive method has a slightly different redshift dependence than that of the algebraic method. The step features in Figure 5 for the naive method arise from discrete changes in the number of steps needed to find  $R_{\text{NL}}$ . On the other hand, the timing of the algebraic method slightly improves with redshift, as at high  $z$  we fit fewer points to determine the polynomial coefficients.

## 5 CONCLUSIONS

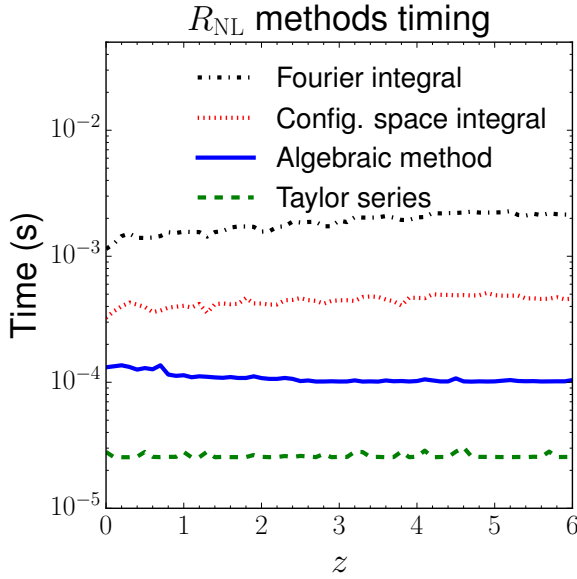
The nonlinear mass is the characteristic scale of halo formation, defined as the scale on which  $\sigma_R$ , the rms of the density field inside a sphere of radius  $R$ , reaches the linear threshold for spherical collapse,  $\delta_c = 1.686$ . We present a method to accelerate computation of the nonlinear mass by an order of magnitude by fitting a polynomial to the correlation function and evaluating  $\sigma_R$  in configuration space. Our method can be further accelerated by a factor of 4 by using a Taylor series about the *Planck* 2018 cosmology for the correlation function fitting coefficients. We make our python implementation publicly available at <https://github.com/akrolewski/NonlinearMassFaster>.

Overall, our method is sufficiently accurate for future applications, with accuracy in the nonlinear mass generally exceeding 1% at  $z < 6$  for a variety of cosmologies. The accuracy is better at lower redshift, where  $R_{\text{NL}}$  is larger and thus depends on the power spectrum at lower  $k$ , where it is less sensitive to cosmological parameters.

A fast and accurate method to compute nonlinear mass will enable repeated calculations of the nonlinear mass. This would be necessary in an MCMC chain for cosmological

<sup>10</sup> Changing  $\Omega_m$  and  $n_s$  tilts  $P(k)$  with a pivot at  $k \approx 0.1 h \text{ Mpc}^{-1}$ . Therefore, the linear power spectrum is more sensitive to cosmological parameters at higher  $k$ .





**Figure 5.** Comparison between the timing for our implementation of the algebraic method (blue) versus the numerical integration plus root-finding method either in Fourier space (black) or configuration space (red). We also show the timing of our method if we instead use a Taylor expansion to generate the coefficients rather than fit them to the correlation function (green). The algebraic method is 10–20 $\times$  faster than the naive method with the integral in Fourier space, and the Taylor series method is 40–80 $\times$  faster.

analysis of a current or upcoming dataset such as DES, DESI or LSST. With this method one could simultaneously vary the nonlinear mass and the cosmology in cosmological inference from the nonlinear regime, potentially enabling more complex modeling to extract cosmological information from smaller scales.

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